

One-dimensional Advection/Diffusion Passive Scalar

1 Introduction

This case provides a description for one-dimensional time advancement of a passive scalar, i.e., constant velocity, whose partial differential equation (PDE) includes the effects of advection and diffusion.

2 Domain

The simple two-dimensional geometry for this tutorial is captured in Figure 1 where the key length of the domain is unity.

The left and right surfaces are periodic while all other surfaces are zero flux. A constant velocity of $u_x = 1$ is applied to the scalar transport equation. A viscosity, ν , is specified to be 0.01, resulting in a Peclet number of 100 based on the domain length and unity based on the local mesh spacing ($Pe = UL/\nu$). The initial condition is simply a Gaussian distribution, see `/src/user_functions/ScalarGaussianAuxFunction.C`.

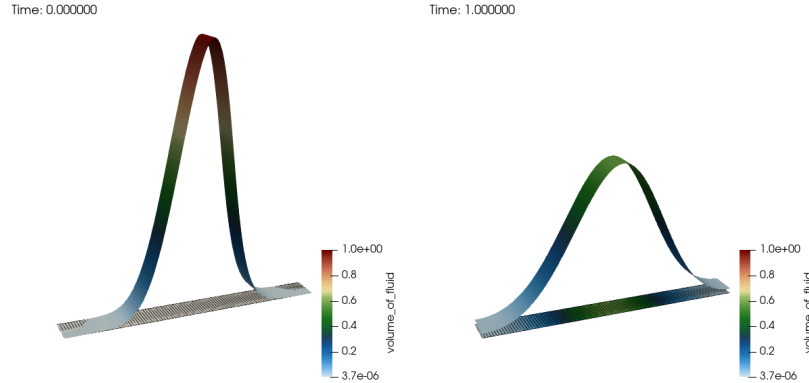


Figure 1: Two-dimensional domain capturing a one-dimensional evolution of a passive scalar at the time of 0 and 1.

3 Theory

The time varying transport of scalar ϕ partial differential equation (PDE) is given by,

$$\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} + \frac{\partial q_j}{\partial x_j} = 0, \quad (1)$$

where q_j is the diffusive flux given by,

$$q_j = -\nu \frac{\partial \phi}{\partial x_j}. \quad (2)$$

3.1 Simulation Specification and Results

The mesh exercised activates a Quad4 topology, thereby exercising a linear basis that yields a nominal second-order spatial accurate simulation. A second-order in time BDF2 three state scheme, which is activated via the "second_order_accuracy" line command, is applied for a fully implicit temporal evolution. Setting this option to "no" yields a first-order Backward Euler time integration. Note that the simulation can be extended in time by increasing the "termination_step_count" setting, or switching this to a physical time, "termination_time". In this mesh configuration, the periodic boundary condition specification mimics an infinitely long domain (left and right boundaries). The top and bottom boundaries are zero-flux, and zero mass injection.

3.1.1 Input Parameters

In the baseline Nalu simulation, the precise PDE definition is achieved through the activation of "element_source_terms" that, for example, activates a time term via "lumped_mass", an advection term via "scs_upw_advection_np", and a diffusion term via "diffusion". The time derivative options in the code base are as follows:

- lumped_mass
- mass

The primary advection term options in the code base allow for either a volume- or surface-based integration:

- scv_advection_np, or $\int u_j \frac{\partial \phi}{\partial x_j} dV$
- scs_advection_np, or $\int u_j \frac{\partial \phi}{\partial x_j} dV = \int \frac{\partial u_j \phi}{\partial x_j} dV - \int \phi \frac{\partial u_j}{\partial x_j} dV$ that for the case of a constant velocity (along with using the Gauss Divergence theorem) can be written as, $\int u_j \phi n_j dS$.

Above, the scs and scv abbreviations represent the sub-control surface and sub-control volume integration points, respectively. For the scs approach, we also allow for an "upwinded" approach through the option, `scs_upw_advection_np`. Here, either an unstructured gradient reconstruction scheme is used (when `upw_factor` is unity), or pure first-order upwind when `upw_factor` is zero). Finally, a limiter for the higher-order upwind scheme can be specified in the limiter setting. Many of the details regarding the meaning of these options will be discussed in upcoming tutorials and laboratory sessions.

4 Discussion Points

There are several interesting activities associated with this sample case including the following:

- Explore the mesh and input file specifications associated with this case.
- Explore the specification of viscosity: increasing and decreasing the nominal value by 10x. What do you see?
- The current advection operator is specified as `"scs_upw_advection_np"`. What happens if you activate `"scs_advection_np"`, again in the context of modification of the viscosity by 10x?
- What happens when viscosity is set to zero?
- Based on what you have learned in class, what is the controlling numerical principle?